Mixing UTA and Detailed Line Treatment for Mid-Z Opacity Calculations

Stephane Mazevet and Joseph Abdallah, Jr., T-4

Current opacity calculations fall in two categories. A detailed line treatment where each transition is calculated explicitly and included in the opacity calculation or a statistical treatment, also known as UTA, where groups of lines belonging to the same transition array are approximated as a single Gaussian. In some applications, the latter method is improved by using random lines in addition to the UTA. The advantages and limitations of each approach is illustrated in Fig. 1 for the $3s^2 3p^3 3d^1 \rightarrow 3s^2 3p^2 3d^3$ transition in argon. Figure 1 shows that this transition involves a total of 2190 individual transitions with oscillator strengths spanning 8 orders of magnitude. Accounting for the total number of lines in an opacity calculation is not efficient as the number of lines and the complexity of the configurations involved increases with the atomic number Z of the element considered and rapidly overcome the computational capabilities. Despite providing a significant simplification as the set of lines is now represented by a single Gaussian, the UTA treatment is not satisfactory either as the loss of spectral accuracy results in a significant uncertainty in the resulting opacity calculation as can be anticipated from the results shown in Fig. 1.

The ATOMIC opacity code is currently based on a detailed line treatment of the atomic spectra to calculate both the Rosseland and Planck opacities. This improved accounting of the various atomic transitions calculated within the detailed *JJ* coupling scheme by the CATS atomic structure codes allows for an improved description of the light element atomic spectra and opacities over the legacy code LEDCOP. This approach is however expensive computationally and can only be realistically applied to light element opacity calculations.

As only a few lines with the largest oscillator strengths are needed to reproduce the spectral structure, we have developed an algorithm to automatically mix the two methods by preserving a detailed treatment for the strongest lines and represent the weakest ones by a UTA. Figure 2 illustrates the usefulness of the method, named MUTA, for the $3s^1 3p^3 3d^2 \rightarrow 3s^1 3p^2 3d^3$ transition in argon. The transition array contains a total of 69424 lines that needs to be included in the opacity calculation. The spectra resulting from the inclusion of these detailed lines is rather structured and would not be well approximated by a Gaussian. Figure 2 shows that a similar spectral accuracy can be obtained by including the 754 strongest lines and including the contribution of the remaining ones using a UTA. Figure 2 shows that the resulting spectra is graphically almost indistinguishable from the original one calculated using the 69424 lines with a saving of almost a factor of a hundred in computational time and disk storage. Additional calculations on MoXV and PrXXXII also indicate that the algorithm developed results in a significant saving for cases where the fine structure splitting and relativistic effects are important.

We show here that a similar accuracy in spectral and opacity calculation can be obtained by mixing a detailed line treatment for the strongest lines with a statistical treatment for the weak ones compared to a full detailed treatment for the same transition array. By reducing the number of detailed lines to be accounted for by about an order of magnitude, the procedure first allows for an equivalent reduction of the amount of memory, disk space, and CPU time needed for a single opacity

calculation. As the method preserves the strongest atomic lines, it is expected that it will result in an improved opacity calculation for mid Z elements where only pure UTA opacity calculations are currently available. The method is currently implemented in CATS, the Los Alamos atomic structure code used to produce the atomic data input for the opacity code ATOMIC to produce a full opacity calculation.

For more information contact Stephane Mazevet at smazevet@lanl.gov.

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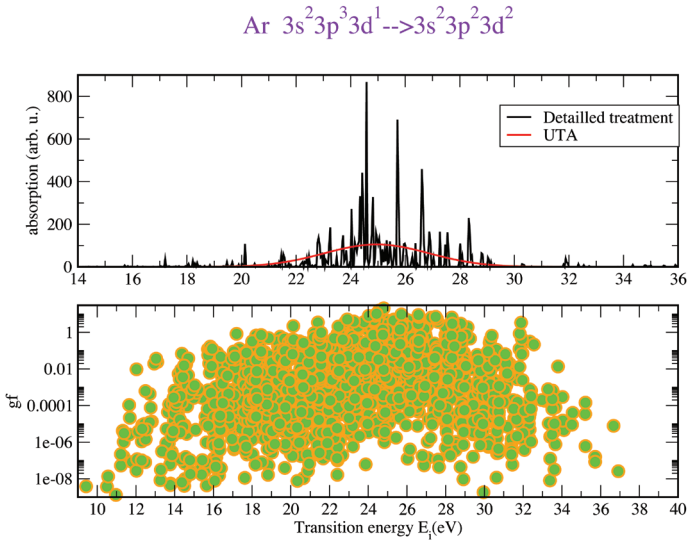

Fig. 1.
(a) Comparison between the detailed and UTA treatment for the $3s^23p^33d^1 \rightarrow 3s^23p^23d^3$ transition in argon. (b) Oscillator strength as a function of transition energies for the same transition.

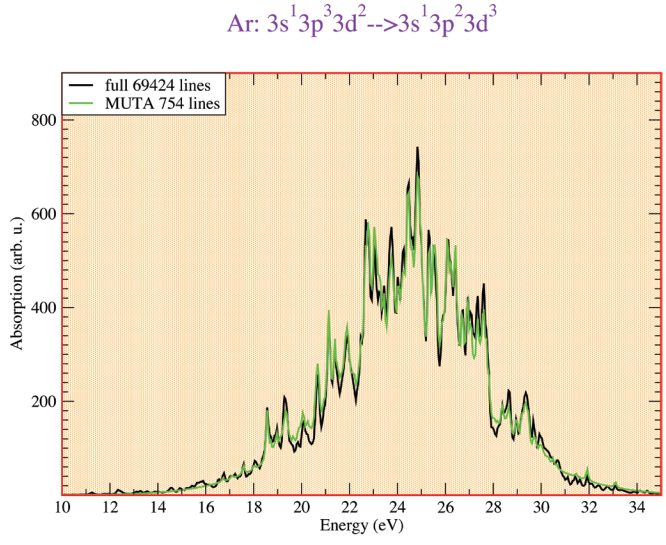

Fig. 2.
(a) MUTA treatment for the $3s^13p^33d^2 \rightarrow 3s^13p^23d^3$ transition in argon.